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NEWS 5 JUL 02 CA/CAPLUS enhanced with utility model patents from China  
NEWS 6 JUL 16 CAPLUS enhanced with French and German abstracts  
NEWS 7 JUL 18 CA/CAPLUS patent coverage enhanced  
NEWS 8 JUL 26 USPATT/PATL/PAT2 enhanced with IPC reclassification  
NEWS 9 JUL 30 USGENE now available on STN  
NEWS 10 AUG 06 CAS REGISTRY enhanced with new experimental property tags  
NEWS 11 AUG 06 BEILSTEIN updated with new compounds  
NEWS 12 AUG 06 PSTA enhanced with new thesaurus edition  
NEWS 13 AUG 13 CA/CAPLUS enhanced with additional kind codes for granted patents  
NEWS 14 AUG 20 CA/CAPLUS enhanced with CAS indexing in pre-1907 records  
NEWS 15 AUG 27 Full-text patent databases enhanced with predefined patent family display formats from INPADOCDB  
NEWS 16 AUG 27 USPATTOLD now available on STN  
NEWS 17 AUG 28 CAS REGISTRY enhanced with additional experimental spectral property data  
NEWS 18 SEP 07 STN AnaVist, Version 2.0, now available with Derwent World Patents Index  
NEWS 19 SEP 13 FORIS renamed to SIFIS  
NEWS 20 SEP 13 INPADOCDB enhanced with monthly SDI frequency  
NEWS 21 SEP 17 CA/CAPLUS enhanced with printed CA page images from 1967-1998  
NEWS 22 SEP 17 CAPLUS coverage extended to include traditional medicine patents

NEWS EXPRESS 19 SEPTEMBER 2007: CURRENT WINDOWS VERSION IS V8.2, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0c(JP), AND CURRENT DISCOVER FILE IS DATED 19 SEPTEMBER 2007.

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FILE COVERS 1907 - 21 Sep 2007 VOL 147 ISS 14  
FILE LAST UPDATED: 20 Sep 2007 (20070920/ED)

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L3 15 L2

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26210138 PY<2006  
L4 11 L3 AND PY<2006

=> d bib abs hitser tot

L4 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2007 ACS ON STN

ACCESSION NUMBER: 2005:979639 CAPLUS

DOCUMENT NUMBER: 143:286443

TITLE: Preparation of pyrimidine derivatives as 5-HT<sub>3</sub> receptor antagonists having agonistic activity on 5-HT<sub>1A</sub>

INVENTOR(S): Sato, Michitaka; Matsui, Teruaki; Asagarsu, Akira; Hayashi, Hiroyuki; Araki, Seichi; Tamaoki, Satoru; Takahashi, Nobuyuki; Yamauchi, Yukinao; Yamamoto, Yoshiko; Yamamoto, Norio; Ogawa, Chisato

SOURCE: Teikoku Hormone Mfg. Co., Ltd., Japan

PCT Int. Appl., 261 pp.

CODEN: PIXX2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WD 2005082887	A1	20050909	WO 2005-JP1691	20050225
W:	AB, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, GU, HK, IL, IN, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, ME, MG, MK, MN, MW, MX, MY, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BM, CH, CM, KE, LG, MW, NZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,			

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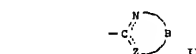
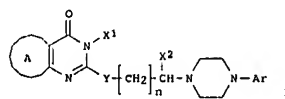
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ER, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CP, CO, CI, CM, GA, GN, GQ, OM, ML, MK, NE, SN, TD, TG  
AU 2005217320 A1 20050909 AU 2005-217320 20050225 --  
CA 2557541 A1 20050909 CA 2005-2557541 20050225 --  
EP 1724267 A1 20061122 EP 2005-719969 20050225  
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, EG, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR  
CN 1922171 A 20070228 CN 2005-80005603 20050225  
US 2007197551 A1 20070823 US 2006-590707 20060825  
PRIORITY APPLN. INFO.: JP 2004-52040 A 20040226  
JP 2004-322858 A 20041105  
WO 2005-JP3691 W 20050225

OTHER SOURCE(S): MARPAT 143:286443

GI



AB Title compds. I (ring A = carbocyclic group, etc.; X1 = H, amino, etc.; X2 = H, alkyl, Y = bond, etc.; n = 0-4; Ar = optionally substituted II with halo, etc.; Z = O, etc.; B = moiety required for completing mono-, ploy-heterocyclic ring containing N together with N-C-Z; dotted line indicates single, double bond were prepared. For example, treatment of potassium 3-amino-5,6-dimethyl-4-oxo-3,4-dihydrothieno[2,3-d]pyrimidine-2-thiolate with 2-(4-(3-chloropropyl)piperazin-1-yl)quinoline, e.g., prepared from piperazine in 2 steps, afforded 3-amino-5,6-dimethyl-2-[(3-(4-quinolin-2-yl)piperazin-1-yl)propylthio]-3H-thieno[2,3-d]pyrimidin-4-one (III) in 50% yield. In 5-HT<sub>3</sub> receptor affinity assay (in vitro), compound III exhibited the antagonistic activity of 94% at 10<sup>-7</sup> M. Compds. I are claimed useful for the treatment of anxiety, depression, etc. Formulation is given.

IT 864385-05-7P 864385-12-6P 864385-49-9P  
864385-51-3P 864385-58-0P 864385-61-5P  
864385-71-7P 864385-72-8P  
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BTOL (Biological study); PNEP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(preparation of pyrimidine derivs. as 5-HT<sub>3</sub> receptor antagonists having agonistic activity on 5-HT<sub>1A</sub> for treatment of anxiety, depression, etc.)

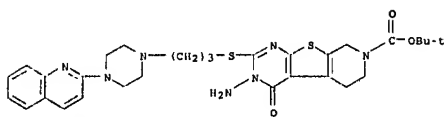
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CN Pyrido[4',3':4,5]thieno[2,3-d]pyrimidine-7(4H)-carboxylic acid, 3-amino-3,5,6,8-tetrahydro-4-oxo-2-[[3-(4-(2-quinolinyl)-1-

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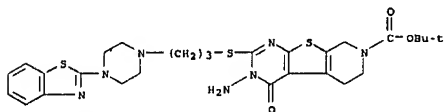
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piperazinylpropylthio)-, 1,1-dimethylethyl ester (CA INDEX NAME)



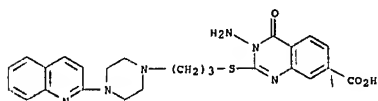
RN 864385-12-6 CAPLUS

CN Pyrido[4',3':4,5]thieno[2,3-d]pyrimidine-7(4H)-carboxylic acid, 3-amino-2-[[3-[(4-(2-benzothiazolyl)-1-piperazinyl)propyl]thio]-3,5,6,8-tetrahydro-4-oxo-, 1,1-dimethylethyl ester (CA INDEX NAME)



RN 864385-49-9 CAPLUS

CN 7-Quinazolinecarboxylic acid, 3-amino-3,4-dihydro-4-oxo-2-[[3-[(4-(2-quinolinyl)-1-piperazinyl)propyl]thio]- (CA INDEX NAME)



RN 864385-51-3 CAPLUS

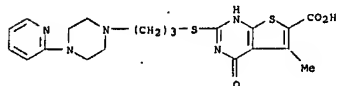
CN Pyrido[4',3':4,5]thieno[2,3-d]pyrimidin-4(3H)-one, 3-amino-5,6,7,8-tetrahydro-2-[[3-[(4-(2-quinolinyl)-1-piperazinyl)propyl]thio]-, trihydrochloride (9CI) (CA INDEX NAME)

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CN Thieno[2,3-d]pyrimidine-6-carboxylic acid, 1,4-dihydro-5-methyl-4-oxo-2-[[3-[(4-(2-pyridinyl)-1-piperazinyl)propyl]thio]- (CA INDEX NAME)



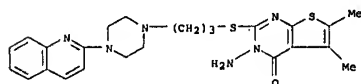
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 864386-74-3P 864386-75-4P 864387-02-0P  
 864387-03-1P 864387-04-2P 864387-05-3P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(Preparation of pyrimidine derivs. as 5-HT<sub>3</sub> receptor antagonists having agonistic activity on 5-HT<sub>1A</sub> for treatment of anxiety, depression, etc.)

RN 864384-93-0 CAPLUS

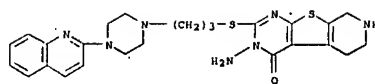
CN Thieno[2,3-d]pyrimidin-4(3H)-one, 3-amino-5,6-dimethyl-2-[[3-[(4-(2-quinolinyl)-1-piperazinyl)propyl]thio]- (CA INDEX NAME)



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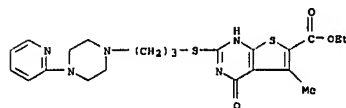
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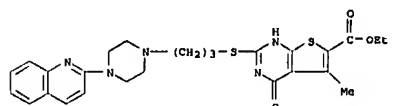
RN 864385-58-0 CAPLUS

CN Thieno[2,3-d]pyrimidine-6-carboxylic acid, 1,4-dihydro-5-methyl-4-oxo-2-[[3-[(4-(2-pyridinyl)-1-piperazinyl)propyl]thio]-, ethyl ester (CA INDEX NAME)



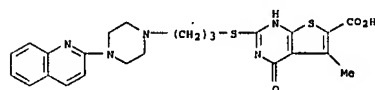
RN 864385-61-5 CAPLUS

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RN 864385-71-7 CAPLUS

CN Thieno[2,3-d]pyrimidine-6-carboxylic acid, 1,4-dihydro-5-methyl-4-oxo-2-[[3-[(4-(2-quinolinyl)-1-piperazinyl)propyl]thio]- (CA INDEX NAME)



RN 864385-72-8 CAPLUS

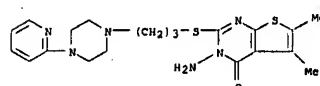
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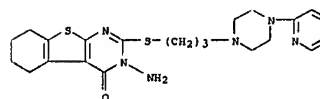
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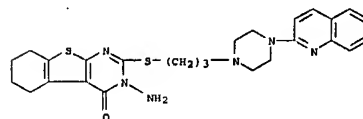
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CN [1]Benzo[thieno[2,3-d]pyrimidin-4(3H)-one, 3-amino-5,6,7,8-tetrahydro-2-[[3-[(4-(2-pyridinyl)-1-piperazinyl)propyl]thio]- (CA INDEX NAME)



RN 864384-96-3 CAPLUS

CN [1]Benzo[thieno[2,3-d]pyrimidin-4(3H)-one, 3-amino-5,6,7,8-tetrahydro-2-[[3-[(4-(2-quinolinyl)-1-piperazinyl)propyl]thio]- (CA INDEX NAME)



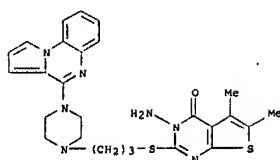
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CN Thieno[2,3-d]pyrimidin-4(3H)-one, 3-amino-5,6-dimethyl-2-[[3-[(4-pyrrolo[1,2-a]quinoxalin-4-yl)-1-piperazinyl)propyl]thio]- (CA INDEX NAME)

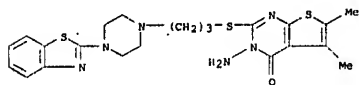
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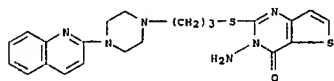
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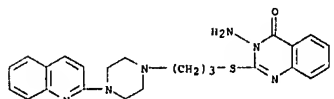
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CN Thieno[2,3-d]pyrimidin-4(3H)-one, 3-amino-2-[[3-[(4-benzothiazolyl)-1-piperazinyl]propylthio]-5,6-dimethyl- (CA INDEX NAME)



RN 864384-99-6 CAPLUS  
CN Thieno[2,3-d]pyrimidin-4(3H)-one, 3-amino-2-[[3-[(4-quinolinyl)-1-piperazinyl]propylthio]- (CA INDEX NAME)



RN 864385-00-2 CAPLUS  
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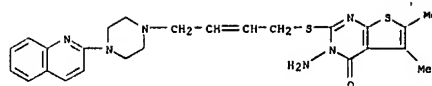


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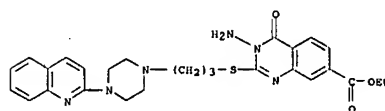
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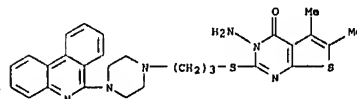
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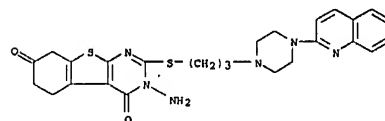
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RN 864385-03-5 CAPLUS  
CN Thieno[2,3-d]pyrimidin-4(3H)-one, 3-amino-5,6-dimethyl-2-[[3-[(4-6-phenanthridinyl)-1-piperazinyl]propylthio]- (CA INDEX NAME)



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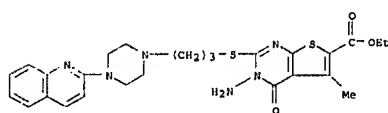


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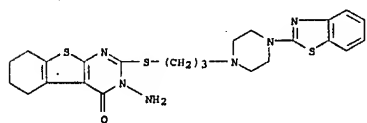
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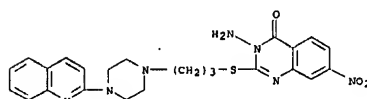
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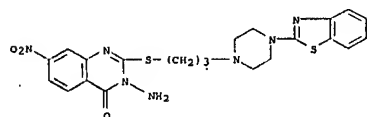
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CN 4(3H)-Quinazolinone, 3-amino-7-nitro-2-[[3-[(4-2-quinolinyl)-1-piperazinyl]propylthio]- (CA INDEX NAME)



RN 864385-09-1 CAPLUS  
CN 4(3H)-Quinazolinone, 3-amino-2-[[3-[(4-2-benzothiazolyl)-1-piperazinyl]propylthio]-7-nitro- (CA INDEX NAME)

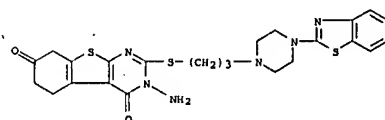


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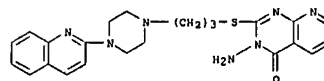
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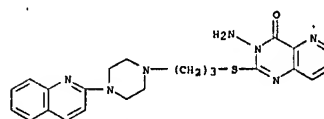
RN 864385-10-4 CAPLUS  
CN [1]Benzothieno[2,3-d]pyrimidine-4,7-dione, 3-amino-2-[[3-[(4-2-benzothiazolyl)-1-piperazinyl]propylthio]-3,5,6,8-tetrahydro- (CA INDEX NAME)



RN 864385-11-5 CAPLUS  
CN Pyrido[2,3-d]pyrimidin-4(3H)-one, 3-amino-2-[[3-[(4-2-quinolinyl)-1-piperazinyl]propylthio]- (CA INDEX NAME)



RN 864385-13-7 CAPLUS  
CN Pyrido[2,3-d]pyrimidin-4(3H)-one, 3-amino-2-[[3-[(4-2-quinolinyl)-1-piperazinyl]propylthio]- (CA INDEX NAME)

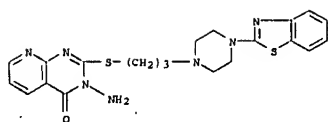


RN 864385-14-8 CAPLUS  
CN Pyrido[2,3-d]pyrimidin-4(3H)-one, 3-amino-2-[[3-[(4-2-benzothiazolyl)-1-piperazinyl]propylthio]- (CA INDEX NAME)

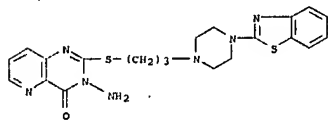
&lt;12/04/2007&gt;

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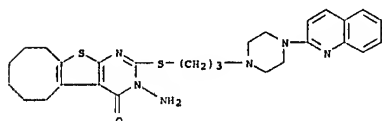
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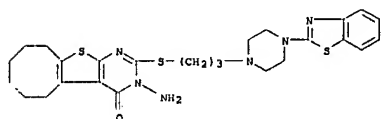
RN 864385-15-9 CAPLUS  
CN Pyrido[3,2-d]pyrimidin-4(3H)-one, 3-amino-2-([3-[4-(2-benzothiazolyl)-1-piperazinyl]propyl]thio)- (CA INDEX NAME)



RN 864385-16-0 CAPLUS  
CN Cycloocta[4,5]thieno[2,3-d]pyrimidin-4(3H)-one, 3-amino-5,6,7,8,9,10-hexahydro-2-([3-[4-(2-quinolinyl)-1-piperazinyl]propyl]thio)- (CA INDEX NAME)



RN 864385-17-1 CAPLUS  
CN Cycloocta[4,5]thieno[2,3-d]pyrimidin-4(3H)-one, 3-amino-2-([3-[4-(2-benzothiazolyl)-1-piperazinyl]propyl]thio)-5,6,7,8,9,10-hexahydro- (CA INDEX NAME)

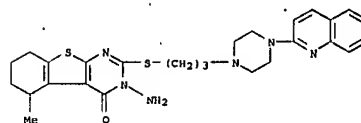


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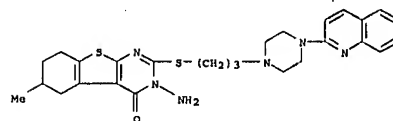
Erich Leese

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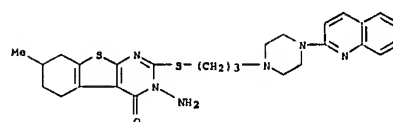
RN 864385-21-7 CAPLUS  
CN [1]Benzo[thieno[2,3-d]pyrimidin-4(3H)-one, 3-amino-5,6,7,8-tetrahydro-6-methyl-2-([3-[4-(2-quinolinyl)-1-piperazinyl]propyl]thio)- (CA INDEX NAME)



RN 864385-22-8 CAPLUS  
CN [1]Benzo[thieno[2,3-d]pyrimidin-4(3H)-one, 3-amino-5,6,7,8-tetrahydro-6-methyl-2-([3-[4-(2-quinolinyl)-1-piperazinyl]propyl]thio)- (CA INDEX NAME)



RN 864385-23-9 CAPLUS  
CN [1]Benzo[thieno[2,3-d]pyrimidin-4(3H)-one, 3-amino-5,6,7,8-tetrahydro-7-methyl-2-([3-[4-(2-quinolinyl)-1-piperazinyl]propyl]thio)- (CA INDEX NAME)

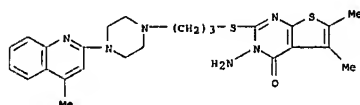


RN 864385-24-0 CAPLUS  
CN Thieno[2,3-d]pyrimidin-4(3H)-one, 3-amino-5,6-dimethyl-2-([3-[4-(4-methyl-2-quinolinyl)-1-piperazinyl]propyl]thio)- (CA INDEX NAME)

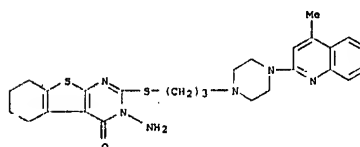
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Erich Leese

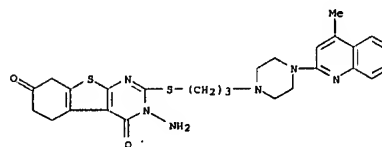
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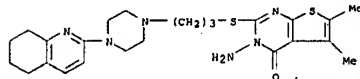
RN 864385-25-1 CAPLUS  
CN [1]Benzo[thieno[2,3-d]pyrimidin-4(3H)-one, 3-amino-5,6,7,8-tetrahydro-2-([3-[4-(4-methyl-2-quinolinyl)-1-piperazinyl]propyl]thio)- (CA INDEX NAME)



RN 864385-26-2 CAPLUS  
CN [1]Benzo[thieno[2,3-d]pyrimidin-4(3H)-one, 3-amino-3,5,6,8-tetrahydro-2-([3-[4-(4-methyl-2-quinolinyl)-1-piperazinyl]propyl]thio)- (CA INDEX NAME)



RN 864385-27-3 CAPLUS  
CN Thieno[2,3-d]pyrimidin-4(3H)-one, 3-amino-5,6-dimethyl-2-([3-[4-(5,6,7,8-tetrahydro-2-quinolinyl)-1-piperazinyl]propyl]thio)- (CA INDEX NAME)

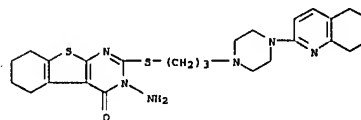


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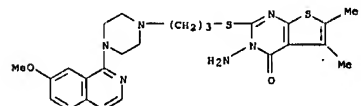
Erich Leese

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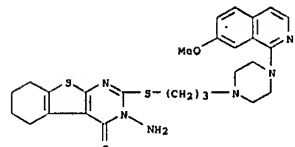
RN 864385-28-4 CAPLUS  
CN [1]Benzo[thieno[2,3-d]pyrimidin-4(3H)-one, 3-amino-5,6,7,8-tetrahydro-2-([3-[4-(5,6,7,8-tetrahydro-2-quinolinyl)-1-piperazinyl]propyl]thio)- (CA INDEX NAME)



RN 864385-30-8 CAPLUS  
CN Thieno[2,3-d]pyrimidin-4(3H)-one, 3-amino-2-([3-[4-(7-methoxy-1-isoquinolinyl)-1-piperazinyl]propyl]thio)-5,6-dimethyl- (CA INDEX NAME)



RN 864385-31-9 CAPLUS  
CN [1]Benzo[thieno[2,3-d]pyrimidin-4(3H)-one, 3-amino-5,6,7,8-tetrahydro-2-([3-[4-(7-methoxy-1-isoquinolinyl)-1-piperazinyl]propyl]thio)- (CA INDEX NAME)

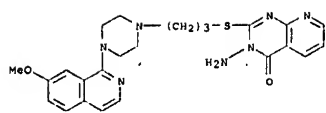


RN 864385-32-0 CAPLUS  
CN Pyrido[2,3-d]pyrimidin-4(3H)-one, 3-amino-2-([3-[4-(7-methoxy-1-isoquinolinyl)-1-piperazinyl]propyl]thio)- (CA INDEX NAME)

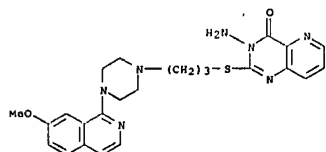
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Erich Leese

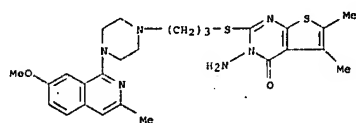
10/513699



RN 864385-33-1 CAPLUS  
CN Pyrido[3,2-d]pyrimidin-4(3H)-one, 3-amino-2-([3-(4-(7-methoxy-1-isoquinolinyl))-1-piperazinyl]propyl)thio- (CA INDEX NAME)



RN 864385-34-2 CAPLUS  
CN Thieno[2,3-d]pyrimidin-4(3H)-one, 3-amino-2-([3-(4-(7-methoxy-3-methyl-1-isoquinolinyl))-1-piperazinyl]propyl)thio-5,6-dimethyl- (CA INDEX NAME)

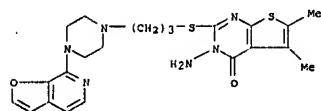


RN 864385-35-3 CAPLUS  
CN [1]Benzo[thieno[2,3-d]pyrimidin-4(3H)-one, 3-amino-5,6,7,8-tetrahydro-2-([3-(4-(7-methoxy-3-methyl-1-isoquinolinyl))-1-piperazinyl]propyl)thio- (CA INDEX NAME)

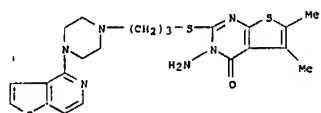
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Erich Leese

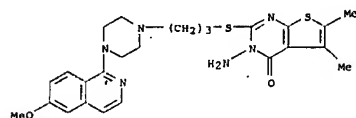
10/513699



RN 864385-39-7 CAPLUS  
CN Thieno[2,3-d]pyrimidin-4(3H)-one, 3-amino-2-([3-(4-furo[3,2-c]pyridin-4-yl-1-piperazinyl]propyl)thio)-5,6-dimethyl- (CA INDEX NAME)



RN 864385-40-0 CAPLUS  
CN Thieno[2,3-d]pyrimidin-4(3H)-one, 3-amino-2-([3-(4-(6-methoxy-1-isoquinolinyl))-1-piperazinyl]propyl)thio-5,6-dimethyl- (CA INDEX NAME)

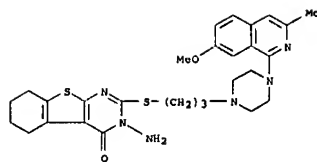


RN 864385-41-1 CAPLUS  
CN [1]Benzo[thieno[2,3-d]pyrimidin-4(3H)-one, 3-amino-5,6,7,8-tetrahydro-2-([3-(4-(6-methoxy-1-isoquinolinyl))-1-piperazinyl]propyl)thio- (CA INDEX NAME)

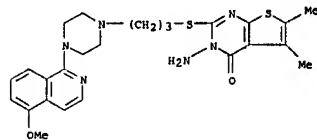
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Erich Leese

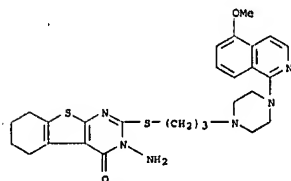
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RN 864385-36-4 CAPLUS  
CN Thieno[2,3-d]pyrimidin-4(3H)-one, 3-amino-2-([3-(4-(5-methoxy-1-isoquinolinyl))-1-piperazinyl]propyl)thio-5,6-dimethyl- (CA INDEX NAME)



RN 864385-37-5 CAPLUS  
CN [1]Benzo[thieno[2,3-d]pyrimidin-4(3H)-one, 3-amino-5,6,7,8-tetrahydro-2-([3-(4-(5-methoxy-1-isoquinolinyl))-1-piperazinyl]propyl)thio- (CA INDEX NAME)

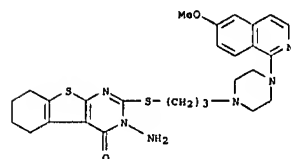


RN 864385-38-6 CAPLUS  
CN Thieno[2,3-d]pyrimidin-4(3H)-one, 3-amino-2-([3-(4-furo[2,3-c]pyridin-7-yl-1-piperazinyl]propyl)thio)-5,6-dimethyl- (CA INDEX NAME)

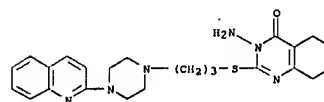
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Erich Leese

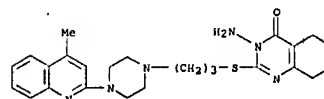
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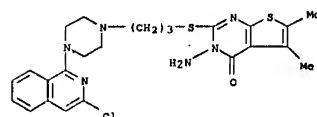
RN 864385-42-2 CAPLUS  
CN 4(3H)-Quinoxalinone, 3-amino-5,6,7,8-tetrahydro-2-([3-(4-(2-quinolinyl))-1-piperazinyl]propyl)thio- (CA INDEX NAME)



RN 864385-43-3 CAPLUS  
CN 4(3H)-Quinoxalinone, 3-amino-5,6,7,8-tetrahydro-2-([3-(4-(4-methyl-2-quinolinyl))-1-piperazinyl]propyl)thio- (CA INDEX NAME)



RN 864385-44-4 CAPLUS  
CN Thieno[2,3-d]pyrimidin-4(3H)-one, 3-amino-2-([3-(4-(3-chloro-1-isoquinolinyl))-1-piperazinyl]propyl)thio-5,6-dimethyl- (CA INDEX NAME)

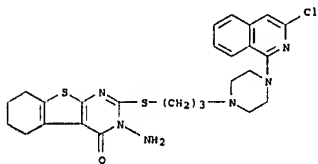


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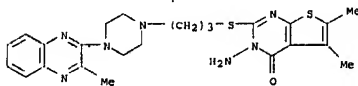
Erich Leese

10/513699

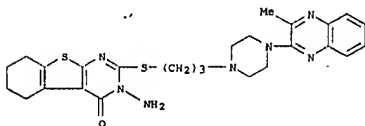
RN 864385-45-5 CAPLUS  
CN [1]Benzo[thieno[2,3-d]pyrimidin-4(3H)-one, 3-amino-2-[[3-[[4-(3-chloro-1-isoquinolyl)-1-piperazinyl]propyl]thio]-5,6,7,8-tetrahydro- (CA INDEX NAME)



RN 864385-46-6 CAPLUS  
CN Thieno[2,3-d]pyrimidin-4(3H)-one, 3-amino-5,6-dimethyl-2-[[3-[[4-(3-methyl-2-quinoxalyl)-1-piperazinyl]propyl]thio]- (CA INDEX NAME)



RN 864385-47-7 CAPLUS  
CN [1]Benzo[thieno[2,3-d]pyrimidin-4(3H)-one, 3-amino-5,6,7,8-tetrahydro-2-[[3-[[4-(3-methyl-2-quinoxalyl)-1-piperazinyl]propyl]thio]- (CA INDEX NAME)



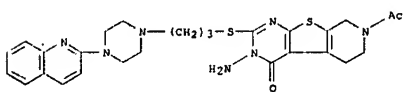
RN 864385-48-8 CAPLUS  
CN Thieno[2,3-d]pyrimidin-4(3H)-one, 3-amino-5,6-dimethyl-2-[[3-[[4-(3-phenyl-2-quinoxalyl)-1-piperazinyl]propyl]thio]- (CA INDEX NAME)

&lt;12/04/2007&gt;

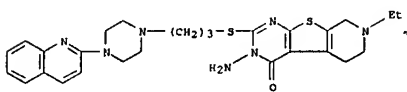
Erich Leese

10/513699

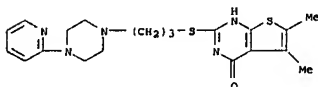
5,6,7,8-tetrahydro-2-[[3-[[4-(2-quinolyl)-1-piperazinyl]propyl]thio]- (CA INDEX NAME)



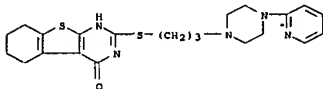
RN 864385-55-7 CAPLUS  
CN Pyrido[4',3':4,5]thieno[2,3-d]pyrimidin-4(3H)-one, 3-amino-7-ethyl-5,6,7,8-tetrahydro-2-[[3-[[4-(2-quinolyl)-1-piperazinyl]propyl]thio]- (CA INDEX NAME)



RN 864385-56-8 CAPLUS  
CN Thieno[2,3-d]pyrimidin-4(1H)-one, 5,6-dimethyl-2-[[3-[[4-(2-pyridinyl)-1-piperazinyl]propyl]thio]- (CA INDEX NAME)



RN 864385-57-9 CAPLUS  
CN [1]Benzo[thieno[2,3-d]pyrimidin-4(1H)-one, 5,6,7,8-tetrahydro-2-[[3-[[4-(2-pyridinyl)-1-piperazinyl]propyl]thio]- (CA INDEX NAME)

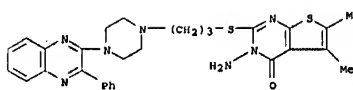


RN 864385-59-1 CAPLUS  
CN Thieno[2,3-d]pyrimidin-4(1H)-one, 5,6-dimethyl-2-[[3-[[4-(2-quinolyl)-1-piperazinyl]propyl]thio]- (CA INDEX NAME)

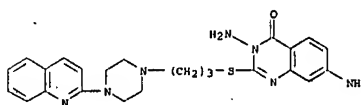
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Erich Leese

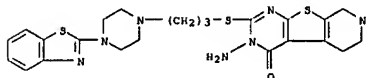
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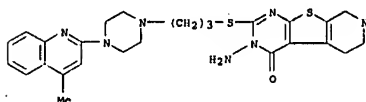
RN 864385-50-2 CAPLUS  
CN 4(3H)-Quinoxalinone, 3,7-diamino-2-[[3-[[4-(2-quinolyl)-1-piperazinyl]propyl]thio]- (CA INDEX NAME)



RN 864385-52-4 CAPLUS  
CN Pyrido[4',3':4,5]thieno[2,3-d]pyrimidin-4(3H)-one, 3-amino-2-[[3-[[4-(2-benzothiazolyl)-1-piperazinyl]propyl]thio]-5,6,7,8-tetrahydro- (CA INDEX NAME)



RN 864385-53-5 CAPLUS  
CN Pyrido[4',3':4,5]thieno[2,3-d]pyrimidin-4(3H)-one, 3-amino-5,6,7,8-tetrahydro-2-[[3-[[4-(4-methyl-2-quinolyl)-1-piperazinyl]propyl]thio]-, trihydrochloride (9CI) (CA INDEX NAME)



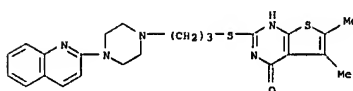
● 3 HCl

RN 864385-54-6 CAPLUS  
CN Pyrido[4',3':4,5]thieno[2,3-d]pyrimidin-4(3H)-one, 7-acetyl-3-amino-

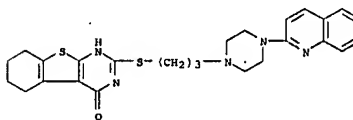
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Erich Leese

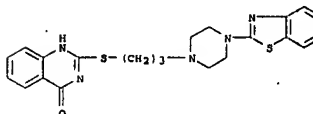
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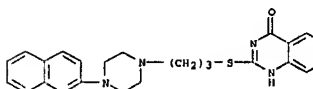
RN 864385-60-4 CAPLUS  
CN [1]Benzo[thieno[2,3-d]pyrimidin-4(1H)-one, 5,6,7,8-tetrahydro-2-[[3-[[4-(2-quinolyl)-1-piperazinyl]propyl]thio]- (CA INDEX NAME)



RN 864385-62-6 CAPLUS  
CN 4(1H)-Quinoxalinone, 2-[[3-[[4-(2-benzothiazolyl)-1-piperazinyl]propyl]thio]- (9CI) (CA INDEX NAME)



RN 864385-63-7 CAPLUS  
CN 4(1H)-Quinoxalinone, 2-[[3-[[4-(2-quinolyl)-1-piperazinyl]propyl]thio]- (9CI) (CA INDEX NAME)



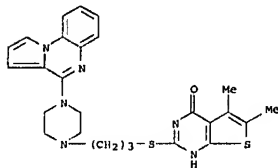
RN 864385-64-8 CAPLUS

&lt;12/04/2007&gt;

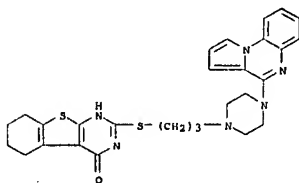
Erich Leese

10/513699

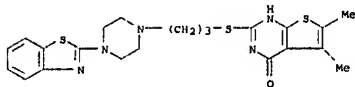
CN Thieno[2,3-d]pyrimidin-4(1H)-one, 5,6-dimethyl-2-[[3-(4-pyrrolo[1,2-a]quinoxalin-4-yl-1-piperazinyl)propyl]thio]- (CA INDEX NAME)



RN 864385-65-9 CAPLUS  
CN (1)Benzo[thieno[2,3-d]pyrimidin-4(1H)-one, 5,6,7,8-tetrahydro-2-[[3-(4-pyrrolo[1,2-a]quinoxalin-4-yl-1-piperazinyl)propyl]thio]- (CA INDEX NAME)



RN 864385-66-0 CAPLUS  
CN Thieno[2,3-d]pyrimidin-4(1H)-one, 2-[[3-[4-(2-benzothiazolyl)-1-piperazinyl]propyl]thio]-5,6-dimethyl- (CA INDEX NAME)

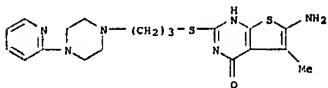


RN 864385-67-1 CAPLUS  
CN Thieno[2,3-d]pyrimidin-4(1H)-one, 2-[[3-[4-(2-quinolinyl)-1-piperazinyl]propyl]thio]- (9CI) (CA INDEX NAME)

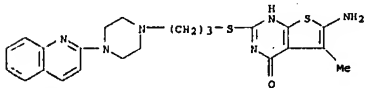
&lt;12/04/2007&gt;

Erich Leese

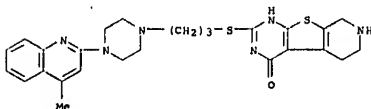
10/513699



RN 864385-74-0 CAPLUS  
CN Thieno[2,3-d]pyrimidin-4(1H)-one, 6-amino-5-methyl-2-[[3-[4-(2-quinolinyl)-1-piperazinyl]propyl]thio]- (CA INDEX NAME)



RN 864385-75-1 CAPLUS  
CN Pyrido[4',3':4,5]thieno[2,3-d]pyrimidin-4(1H)-one, 5,6,7,8-tetrahydro-2-[[3-[4-(4-methyl-2-quinolinyl)-1-piperazinyl]propyl]thio]-, trihydrochloride (9CI) (CA INDEX NAME)



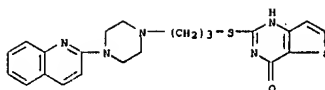
●3 HCl

RN 864385-76-2 CAPLUS  
CN Pyrido[4',3':4,5]thieno[2,3-d]pyrimidin-4(1H)-one, 5,6,7,8-tetrahydro-2-[[3-[4-(4-methyl-2-quinolinyl)-1-piperazinyl]propyl]thio]-, trihydrochloride (9CI) (CA INDEX NAME)

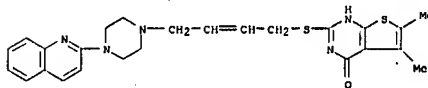
&lt;12/04/2007&gt;

Erich Leese

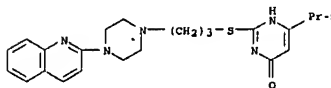
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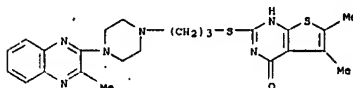
RN 864385-68-2 CAPLUS  
CN Thieno[2,3-d]pyrimidin-4(1H)-one, 5,6-dimethyl-2-[[4-[4-(2-quinolinyl)-1-piperazinyl]-2-butenyl]thio]- (9CI) (CA INDEX NAME)



RN 864385-69-3 CAPLUS  
CN 4(1H)-Pyrimidinone, 6-propyl-2-[[3-[4-(2-quinolinyl)-1-piperazinyl]propyl]thio]- (9CI) (CA INDEX NAME)



RN 864385-70-6 CAPLUS  
CN Thieno[2,3-d]pyrimidin-4(1H)-one, 5,6-dimethyl-2-[[3-[4-(3-methyl-2-quinoxaliny)]-1-piperazinyl]propyl]thio]- (CA INDEX NAME)

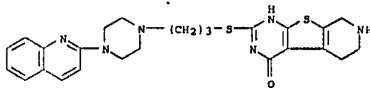


RN 864385-73-9 CAPLUS  
CN Thieno[2,3-d]pyrimidin-4(1H)-one, 6-amino-5-methyl-2-[[3-[4-(2-pyridinyl)-1-piperazinyl]propyl]thio]- (CA INDEX NAME)

&lt;12/04/2007&gt;

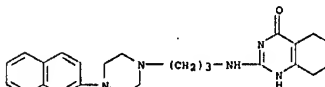
Erich Leese

10/513699

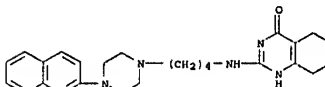


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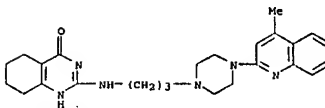
RN 864386-65-2 CAPLUS  
CN 4(1H)-Quinazolinone, 5,6,7,8-tetrahydro-2-[[3-[4-(2-quinolinyl)-1-piperazinyl]propyl]amino]- (9CI) (CA INDEX NAME)



RN 864386-66-3 CAPLUS  
CN 4(1H)-Quinazolinone, 5,6,7,8-tetrahydro-2-[[4-[4-(2-quinolinyl)-1-piperazinyl]butyl]amino]- (9CI) (CA INDEX NAME)



RN 864386-67-4 CAPLUS  
CN 4(1H)-Quinazolinone, 5,6,7,8-tetrahydro-2-[[3-[4-[4-methyl-2-quinolinyl)-1-piperazinyl]propyl]amino]- (9CI) (CA INDEX NAME)



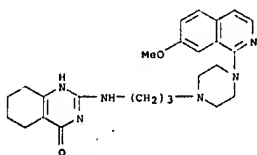
RN 864386-68-5 CAPLUS

&lt;12/04/2007&gt;

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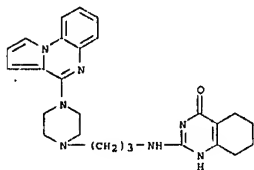
10/513699

CN 4(1H)-Quinazolinone, 5,6,7,8-tetrahydro-2-[[3-[4-(7-methoxy-1-isoquinolinyl)-1-piperazinyl]propyl]amino]- (9CI) (CA INDEX NAME)



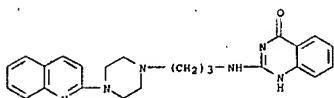
RN 864386-69-6 CAPLUS

CN 4(1H)-Quinazolinone, 5,6,7,8-tetrahydro-2-[[3-(4-pyrrolo[1,2-a]quinoxalin-4-yl-1-piperazinyl)propyl]amino]- (9CI) (CA INDEX NAME)



RN 864386-70-9 CAPLUS

CN 4(1H)-Quinazolinone, 2-[[3-[4-(2-quinolinyl)-1-piperazinyl]propyl]amino]- (CA INDEX NAME)



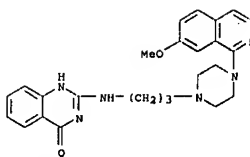
RN 864386-71-0 CAPLUS

CN 4(1H)-Quinazolinone, 2-[[3-[4-(7-methoxy-1-isoquinolinyl)-1-piperazinyl]propyl]amino]- (CA INDEX NAME)

&lt;12/04/2007&gt;

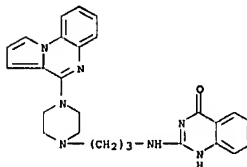
Erich Leese

10/513699



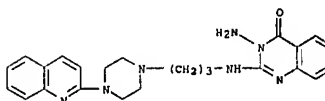
RN 864386-72-1 CAPLUS

CN 4(1H)-Quinazolinone, 2-[[3-(4-pyrrolo[1,2-a]quinoxalin-4-yl-1-piperazinyl)propyl]amino]- (CA INDEX NAME)



RN 864386-73-2 CAPLUS

CN 4(3H)-Quinazolinone, 3-amino-2-[[3-[4-(2-quinolinyl)-1-piperazinyl]propyl]amino]- (CA INDEX NAME)



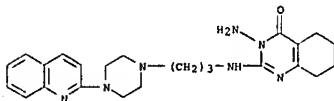
RN 864386-74-3 CAPLUS

CN 4(3H)-Quinazolinone, 3-amino-5,6,7,8-tetrahydro-2-[[3-[4-(2-quinolinyl)-1-piperazinyl]propyl]amino]- (CA INDEX NAME)

&lt;12/04/2007&gt;

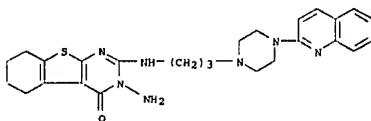
Erich Leese

10/513699



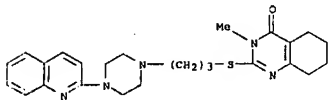
RN 864386-75-4 CAPLUS

CN (1)Benzo[thieno(2,3-d)pyrimidin-4(3H)-one, 3-amino-5,6,7,8-tetrahydro-2-[[3-[4-(2-quinolinyl)-1-piperazinyl]propyl]amino]- (CA INDEX NAME)



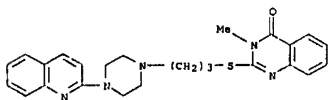
RN 864387-02-0 CAPLUS

CN 4(3H)-Quinazolinone, 5,6,7,8-tetrahydro-3-methyl-2-[[3-[4-(2-quinolinyl)-1-piperazinyl]propyl]thio]- (CA INDEX NAME)



RN 864387-03-1 CAPLUS

CN 4(3H)-Quinazolinone, 3-methyl-2-[[3-[4-(2-quinolinyl)-1-piperazinyl]propyl]thio]- (CA INDEX NAME)



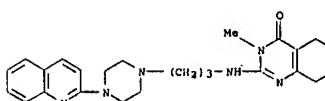
RN 864387-04-2 CAPLUS

CN 4(3H)-Quinazolinone, 5,6,7,8-tetrahydro-3-methyl-2-[[3-[4-(2-quinolinyl)-1-piperazinyl]propyl]amino]- (CA INDEX NAME)

&lt;12/04/2007&gt;

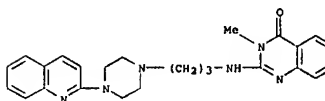
Erich Leese

10/513699



RN 864387-05-3 CAPLUS

CN 4(3H)-Quinazolinone, 3-methyl-2-[[3-[4-(2-quinolinyl)-1-piperazinyl]propyl]thio]- (CA INDEX NAME)



IT 864387-12-2 864387-13-3 864387-14-4

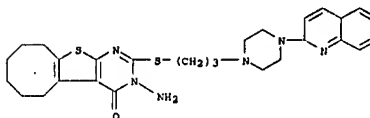
864387-15-5 864387-16-6

RL: PAC (Pharmacological activity), THU (Therapeutic use), BIOL (Biological study); USES (Uses)

(preparation of pyrimidine derivs. as 5-HT<sub>3</sub> receptor antagonists having agonistic activity on 5-HT<sub>1A</sub> for treatment of anxiety, depression, etc.)

RN 864387-12-2 CAPLUS

CN Cycloocta[4,5]thieno[2,3-d]pyrimidin-4(3H)-one, 3-amino-2-[[3-[4-(2,4a-dihydro-2-quinolinyl)-1-piperazinyl]propyl]thio]-5,6,7,8,9,10-hexahydro- (CA INDEX NAME)



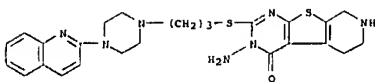
RN 864387-13-3 CAPLUS

CN Pyrido[4',3':4,5]thieno[2,3-d]pyrimidin-4(3H)-one, 3-amino-5,6,7,8-tetrahydro-2-[[3-[4-(2-quinolinyl)-1-piperazinyl]propyl]thio]- (CA INDEX NAME)

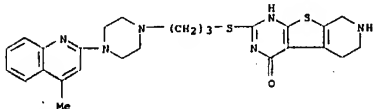
&lt;12/04/2007&gt;

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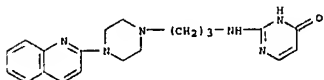




RN 864387-14-4 CAPLUS  
CN Pyrido[4',3':4,5]thieno[2,3-d]pyrimidin-4(1H)-one, 5,6,7,8-tetrahydro-2-[[3-{4-(4-methyl-2-quinolinyl)-1-piperazinyl}propylthio]- (CA INDEX NAME)



RN 864387-15-5 CAPLUS  
CN 4(1H)-Pyrimidinone, 2-[[3-{4-(2-quinolinyl)-1-piperazinyl}propylamino]- (CA INDEX NAME)

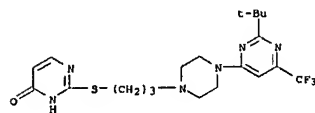


RN 864387-16-6 CAPLUS  
CN 4(1H)-Pyrimidinone, 2-[[3-{4-(2-pyrrolo[1,2-a]quinoxalin-4-yl-1-piperazinyl}propylamino)- (CA INDEX NAME)

&lt;12/04/2007&gt;

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(LU-201640), a selective D3 receptor antagonist (17.46  $\mu\text{mol/kg}$ ), showed a nonsignificant trend to attenuate the effect of the low dose of quinpirole, and L-745,870, a selective D4 receptor antagonist (1.15  $\mu\text{mol/kg}$ ), had no effect. The pharmacol. selectivity of the compds. tested suggests that the antidepressant-like effects of quinpirole are most likely mediated mainly by D2 and to a lesser extent by D3 but not D4 receptors.  
IT 220519-06-2, A 37203  
RL: BSU (Biological study, unclassified); BIOL (Biological study)  
(Lu 201640; D3 receptor antagonist; L-745,870 showed non significant trend to block antidepressant effect of quinpirole in rat model for depression suggest antidepressant effect of quinpirole less likely mediated by D3 receptor)  
RN 220519-06-2 CAPLUS  
CN 4(1H)-Pyrimidinone, 2-[[3-{4-(2-(1,1-dimethylethyl)-6-(trifluoromethyl)-4-pyrimidinyl)-1-piperazinyl}propylthio]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 93 THERE ARE 93 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:348194 CAPLUS

DOCUMENT NUMBER: 140:35302

TITLE: Multiconformational method for analyzing the biological activity of molecular structures

AUTHOR(S): Potemkin, V. A.; Arslambekov, R. M.; Bartashevich, E. V.; Grishina, M. A.; Belik, A. V.; Perspicace, S.; Oucione, S.

CORPORATE SOURCE: Chelyabinsk State University, Chelyabinsk, Russia

SOURCE: Journal of Structural Chemistry (Translation of Zhurnal Strukturnoi Khimii) (2002), 43(6), 1045-1049

CODEN: JSTCAM, ISSN: 0022-4766

PUBLISHER: Kluwer Academic/Consultants Bureau

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A multiconformational method for analyzing the biol. activity of compds. is proposed that combines conformer search algorithms and a 3D-QSAR receptor modeling procedure. The method allows one to find high-activity and low-activity conformers and determine the receptor shape. The biol. activity of a substance is determined as a superposition of the activities of its conformers with allowance for their proportions in the substance. Agreement between calculated and exptl. conformations and between calculated

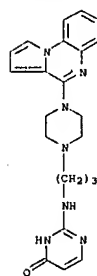
and exptl. biol. activities (pIC50) is demonstrated by the example of agonists of the 5-HT1A receptor.

IT 185202-63-5 185202-78-2 185203-17-2

185203-19-4

&lt;12/04/2007&gt;

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REFERENCE COUNT:

11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:526514 CAPLUS

DOCUMENT NUMBER: 144:121488

TITLE:

Antidepressant-like effect of D2/D3 receptor-, but not D4 receptor-activation in the rat forced swim test. Basso, Ana M.; Gallagher, Kelly B.; Bratcher, Natalie A.; Brioni, Jorge D.; Moreland, Robert B.; Hsieh, Gin C.; Drescher, Karla; Fox, Gerard B.; Decker, Michael W.; Rueter, Lynne E.

CORPORATE SOURCE: Neuroscience Research, Global Pharmaceutical Research & Development, Abbott Laboratories, Abbott Park, IL, USA

SOURCE: Neuropsychopharmacology (2005), 30(7), 1257-1268

CODEN: NEROEW, ISSN: 0893-133X

PUBLISHER: Nature Publishing Group

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Dopamine plays a role in the pathophysiol. of depression and therapeutic effects of antidepressants but the contribution of individual D2-like receptor subtypes (D2, D3, D4) to depression is not known. We present evidence that activation of D2/D3, but not D4 receptors, can affect the outcome in the rat forced swim test (FST). Nomifensine, a dopamine uptake inhibitor (7, 14, and 28  $\mu\text{mol/kg}$ ), quinpirole, a D2-like receptor and agonist (0.4, 1.0, and 2.0  $\mu\text{mol/kg}$ ), PD 12,8907, a preferential D3 receptor agonist (0.17, 0.35, and 0.7  $\mu\text{mol/kg}$ ), PD 168077 (0.1, 0.3, and 1.0  $\mu\text{mol/kg}$ ) and CP 226269 (0.3, 1.0, and 3.0  $\mu\text{mol/kg}$ ), both selective D4 receptor agonists, were administered s.c. 24, 5, and 0.5/1 h before testing. Nomifensine, quinpirole at all doses and PD 128907 at the highest dose decreased immobility time in FST. PD 168077 and CP 226269 had no effect on the model. To further clarify what type of dopamine receptors were involved in the anti-immobility effect of quinpirole, we tested different antagonists. Haloperidol, a D2-like receptor antagonist (0.27  $\mu\text{mol/kg}$ ), completely blocked the effect of quinpirole; A-47203

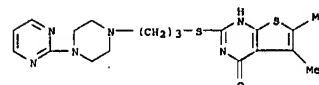
&lt;12/04/2007&gt;

Erich Leese

RL: PAC (Pharmacological activity); BIOL (Biological study)  
(multiconformational method for analyzing the biol. activity of mol. structures)

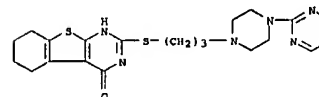
RN 185202-63-5 CAPLUS

CN Thieno[2,3-d]pyrimidin-4(1H)-one, 5,6-dimethyl-2-[[3-{4-(2-pyrimidinyl)-1-piperazinyl}propylthio]- (9CI) (CA INDEX NAME)



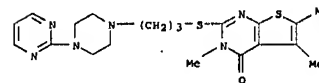
RN 185202-78-2 CAPLUS

CN [1]Benzothieno[2,3-d]pyrimidin-4(1H)-one, 5,6,7,8-tetrahydro-2-[[3-{4-(2-pyrimidinyl)-1-piperazinyl}propylthio]- (9CI) (CA INDEX NAME)



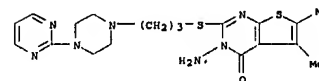
RN 185203-17-2 CAPLUS

CN Thieno[2,3-d]pyrimidin-4(3H)-one, 3,5,6-trimethyl-2-[[3-{4-(2-pyrimidinyl)-1-piperazinyl}propylthio]- (9CI) (CA INDEX NAME)



RN 185203-19-4 CAPLUS

CN Thieno[2,3-d]pyrimidin-4(3H)-one, 3-amino-5,6-dimethyl-2-[[3-{4-(2-pyrimidinyl)-1-piperazinyl}propylthio]- (9CI) (CA INDEX NAME)



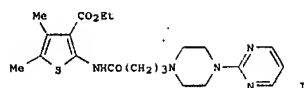
REFERENCE COUNT:

15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

&lt;12/04/2007&gt;

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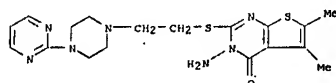
Krich Lease



AB The synthesis and the binding tests on the 5-HT<sub>3</sub> and 5-HT<sub>4</sub> receptors of new thienopyrimidinone and piperazinylacetylaminothienothiopyran derivatives, in order to identify potent and selective ligands for each receptor, is reported. The compound with higher affinity and selectivity for the 5-HT<sub>3</sub> over the 5-HT<sub>4</sub> receptor was the 3-amino-2-(4-benzyl-1-piperazinyl)-5,6-dimethyl-thieno[2,3-d]pyrimidin-4(3H)-one (5-HT<sub>3</sub> K<sub>i</sub> = 3.92 nM, 5-HT<sub>4</sub> not active), the compound with higher affinity and selectivity for the 5-HT<sub>4</sub> over the 5-HT<sub>3</sub> receptor was 2-[4-(2-pyrimidinyl)-1-piperazinyl]butanoylamino-4,5-dimethyl-3-thiophenecarboxylic acid Et ester (1) (5-HT<sub>4</sub> K<sub>i</sub> = 81.3 nM, 5-HT<sub>3</sub> not active). Conformational analyses were carried out on the compds. of the piperazinylacetylaminothienothiopyran series taking 1 as the template.

IT 315275-09-7P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
 (preparation and binding properties of novel and selective 5-HT<sub>3</sub> and 5-HT<sub>4</sub> receptor ligands)

RN 315275-09-7 CAPLUS  
 CN Thieno[2,3-d]pyrimidin-4(3H)-one, 3-amino-5,6-dimethyl-2-[[3-[4-(2-pyrimidinyl)-1-piperazinyl]ethyl]thio]- (9CI) (CA INDEX NAME)

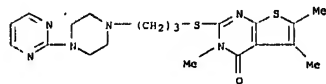


REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

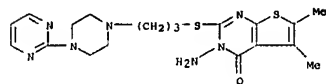
L4 ANSWER 7 OF 11 CAPLUS COPYRIGHT 2007 ACS ON STN  
 ACCESSION NUMBER: 2000:696300 CAPLUS  
 DOCUMENT NUMBER: 133:344185  
 TITLE: 3D-QSAR using "multiconformer" alignment: the use of HASL in the analysis of 5-HT<sub>1A</sub> thienopyrimidinone ligands  
 AUTHOR(S): Guccione, Salvatore; Doweiko, Arthur M.; Chen, Hongming; Barretta, Gloria Uccello; Balzano, Federica  
 CORPORATE SOURCE: Dipartimento di Scienze Farmaceutiche, Università di Catania, Catania, I-95125, Italy  
 SOURCE: Journal of Computer-Aided Molecular Design (2000), 14(7), 647-657  
 CODEN: JCADEQ; ISSN: 0920-654X  
 PUBLISHER: Kluwer Academic Publishers

&lt;12/04/2007&gt;

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RN 185203-19-4 CAPLUS  
 CN Thieno[2,3-d]pyrimidin-4(3H)-one, 3-amino-5,6-dimethyl-2-[[3-[4-(2-pyrimidinyl)-1-piperazinyl]propyl]thio]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 11 CAPLUS COPYRIGHT 2007 ACS ON STN  
 ACCESSION NUMBER: 2000:379673 CAPLUS  
 DOCUMENT NUMBER: 133:171775  
 TITLE: High potent and selective arylpiperazine derivatives as ligands for the 5-HT<sub>1A</sub> receptor  
 AUTHOR(S): Mcdica, Maria; Santagati, Maria; Santagati, Andrea; Russo, Filippo; Cagnotto, Alfredo; Goegan, Mara; Mennini, Tiziana  
 CORPORATE SOURCE: Dipartimento di Scienze Farmaceutiche, Università di Catania, Catania, 95125, Italy  
 SOURCE: Bioorganic & Medicinal Chemistry Letters (2000), 10(10), 1049-1052  
 CODEN: BMCLEB; ISSN: 0960-894X  
 PUBLISHER: Elsevier Science Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB This paper reports the synthesis of new arylpiperazinylalkylthiothienopyrimidine and thiazole derivs. and their affinities for the 5-HT<sub>1A</sub> vs. the 5-HT<sub>2A</sub> receptors. Most of the arylpiperazines show affinities values in the nanomolar range for the 5-HT<sub>1A</sub> receptor. One compound is highly potent (K<sub>i</sub> 0.26 nM, selectivity 28), two other derivs. are less potent, but highly selective (K<sub>i</sub> 9.40 and 5.06 nM, selectivity 207 and 73, resp.).

IT 288591-23-1P 288591-24-2P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation and properties of arylpiperazinylalkylthiothienopyrimidine and -thiazole derivs. and their potency and selectivity as ligands for the 5-HT<sub>1A</sub> receptor)

RN 288591-23-1 CAPLUS  
 CN Thieno[2,3-d]pyrimidin-4(3H)-one, 3-amino-6-ethyl-2-[[3-[4-(2-pyrimidinyl)-1-piperazinyl]propyl]thio]- (9CI) (CA INDEX NAME)

&lt;12/04/2007&gt;

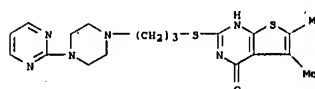
Erich Leese

DOCUMENT TYPE: Journal  
 LANGUAGE: English

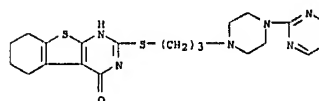
AB The observed 5-HT<sub>1A</sub> and α<sub>1</sub>-adrenergic receptor (α<sub>1</sub>-AR) receptor binding properties of a series of 23 thienopyrimidinones were used to develop HASL 3D-QSAR models. A single, low energy conformer of the most active analog in the series, which was consistent with NMR structural studies, was chosen as a template mol. Alignments of all the mols. to the template were provided by an Amber/MM2 superposition force field. In this manner, each mol. was represented by five sep. low energy conformers which were subsequently used in the generation of HASL 3D-QSAR models. Models derived from multiple conformers were found to exhibit enhanced predictivity compared to models based on single, low energy conformers. In addition, the use of contour imaging of HASL multi-conformer model interactions was found to lead to a more consistent interpretation of those mol. features most significant for 5-HT<sub>1A</sub> receptor binding.

IT 185202-63-5 185202-78-2 185203-17-2  
 185203-19-4  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)  
 (3D-QSAR using "multiconformer" alignment; use of HASL in anal. of 5-HT<sub>1A</sub> thienopyrimidinone ligands)

RN 185202-63-5 CAPLUS  
 CN Thieno[2,3-d]pyrimidin-4(3H)-one, 5,6-dimethyl-2-[[3-[4-(2-pyrimidinyl)-1-piperazinyl]propyl]thio]- (9CI) (CA INDEX NAME)



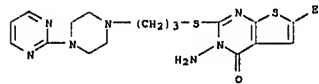
RN 185202-78-2 CAPLUS  
 CN 11-Benzothieno[2,3-d]pyrimidin-4(1H)-one, 5,6,7,8-tetrahydro-2-[[3-[4-(2-pyrimidinyl)-1-piperazinyl]propyl]thio]- (9CI) (CA INDEX NAME)



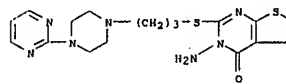
RN 185203-17-2 CAPLUS  
 CN Thieno[2,3-d]pyrimidin-4(3H)-one, 3,5,6-trimethyl-2-[[3-[4-(2-pyrimidinyl)-1-piperazinyl]propyl]thio]- (9CI) (CA INDEX NAME)

&lt;12/04/2007&gt;

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RN 288591-24-2 CAPLUS  
 CN Thieno[2,3-d]pyrimidin-4(3H)-one, 3-amino-2-[[3-[4-(2-pyrimidinyl)-1-piperazinyl]propyl]thio]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 11 CAPLUS COPYRIGHT 2007 ACS ON STN  
 ACCESSION NUMBER: 1999:127124 CAPLUS  
 DOCUMENT NUMBER: 130:182482  
 TITLE: 2-[3-[(4-tert-Butyl-6-trifluoromethylpyrimidin-4-yl)piperazin-1-yl]propyl]thiothienopyrimidin-4-ol fumarate  
 INVENTOR(S): Blank, Stefan; Starck, Dorothea; Treiber, Hans-Joerg; Koser, Stefan; Schaefer, Bernd; Thyse, Marco; Hoeger, Thomas  
 PATENT ASSIGNER(S): BASF A.-G., Germany  
 SOURCE: Ger. Offen., 4 pp.  
 CODEN: GWXBXK  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19735410	A1	19990218	DE 1997-19735410	19970814 <--
TW 467912	B	20011211	TW 1998-87113230	19980812 <--
ZA 9807239	A	20000214	ZA 1998-7239	19980813 <--
TN 1998MA01839	A	20050304	TN 1998-MA01839	19980813 <--
CA 2301297	A1	19990225	CA 1998-2301297	19980814 <--
WO 9909015	A1	19990225	WO 1998-EP5178	19980814 <--
W: AL, AU, BG, BR, BY, CA, CN, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IL, JP, KR, KZ, LT, LV, MK, NO, NZ, PL, RO, RU, SE, SI, SK, TR, UA, US, AM, AZ, KG, MD, TG, TM				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9893426	A	19990308	AU 1998-93426	19980814 <--
AU 749575	B2	20000207		
TR 200000406	T2	20000522	TR 2000-200000406	19980814 <--
EP 1003728	A1	20000531	EP 1998-946343	19980814 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IL, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				

&lt;12/04/2007&gt;

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BR 9811177 A 20000725 BR 1998-11177 19980814 <--  
 NZ 502675 A 20010629 NZ 1998-502675 19980814 <--  
 JP 2001515070 T 20010918 JP 2000-509698 19980814 <--  
 HU 200003710 A2 20011028 HU 2000-3710 19980814 <--  
 IL 134246 A 20021110 IL 1998-134246 19980814 <--  
 MX 200001161 A 20001115 MX 2000-1161 20000202 <--  
 BG 104122 A 20001130 BG 2000-104122 20000203 <--  
 NO 2000000665 A 20000210 NO 2000-665 20000210 <--  
 NO 314935 B1 20030616 20000210 <--  
 US 2001020022 A1 20010906 US 2000-485460 20000210 <--  
 US 2002143179 A1 20021003 US 2002-39974 20020108 <--  
 US 6486162 B2 20021126

## PRIORITY APPLN. INFO.:

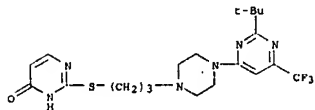
AB The title compound was prepared from the pyrimidine, piperazine, and thiouracil fragments. The fumarate had a half-life in 1N HCl that was >5 times longer than that of the free base, indicating much greater stability to stomach acid for the fumarate.

IT 220519-06-2P

RL: BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
 (preparation and acid stability of 2-[3-[4-(2-(1,1-dimethylethyl)-6-(trifluoromethyl)pyrimidin-4-yl)piperazin-1-yl]propylthio]pyrimidin-4-ol fumarate)

RN 220519-06-2 CAPLUS

CN 4(1H)-Pyrimidinone, 2-[[3-[4-(2-(1,1-dimethylethyl)-6-(trifluoromethyl)-4-pyrimidinyl]-1-piperazinyl)propylthio]- (9CI) (CA INDEX NAME)



IT 220519-07-3P

RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation and acid stability of 2-[3-[4-(2-(1,1-dimethylethyl)-6-(trifluoromethyl)pyrimidin-4-yl)piperazin-1-yl]propylthio]pyrimidin-4-ol fumarate)

RN 220519-07-3 CAPLUS

CN 4(1H)-Pyrimidinone, 2-[[3-[4-(2-(1,1-dimethylethyl)-6-(trifluoromethyl)-4-pyrimidinyl]-1-piperazinyl)propylthio]- (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

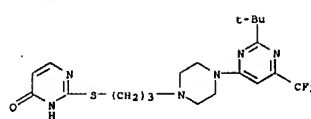
CRN 220519-06-2

CMP C20 H27 F3 N6 O 5

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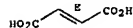


CM 2

CRN 110-17-8

CMP C4 H4 O4

Double bond geometry as shown.



L4 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1997:80137 CAPLUS

DOCUMENT NUMBER: 126:69742

TITLE: 1-((Arylpiperazinyl)alkyl)thiothieno[2,3-d]pyrimidinone Derivatives as High-Affinity, Selective 5-HT1A Receptor Ligands

AUTHOR(S): Modica, Maria; Santagati, Maria; Russo, Filippo; Perocci, Luca; De Giola, Luca; Selvaggini, Carlo; Salmons, Mario; Mennini, Tiziana

CORPORATE SOURCE: Dipartimento di Scienze Farmaceutiche, Università di Catania, Catania, 95125, Italy

SOURCE: Journal of Medicinal Chemistry (1997), 40(4), 574-585

CODEN: JMCWAR, ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A series of 2-[[4-(arylpiperazinyl)alkyl]thiothieno[2,3-d]pyrimidin-4(1H)-one and 3-substituted 2-[[4-(arylpiperazinyl)alkyl]thiothieno[2,3-d]pyrimidin-4(3H)-one] derivatives were prepared and evaluated for in vitro 5-HT1A receptor affinity by radioligand binding assays; the selectivity for 5-HT1A receptors rather than alpha-adrenoceptors was also examined (ratio of the IC50 alpha to IC50 5-HT1A). The binding tests gave indications about the best features of the ((arylpiperazinyl)alkyl)thio moiety and of the substituents on the thiophene and pyrimidinone rings for efficacious and selective 5-HT1A ligands. The most effective derivative for displacing [3H]-8-OH-DPAT from rat hippocampal membranes was 3-amino-2-[[3-[4-(2-methoxyphenyl)-1-piperazinyl]propylthio]-5,6-dimethylthieno[2,3-d]pyrimidin-4(3H)-one (IC50 = 0.3 nM) with selectivity of 24 for the 5-HT1A over the alpha-adrenoceptor. Another compound, where the 2-methoxyphenyl group on the N4 piperazine ring was replaced with a pyrimidinone group, showed the best selectivity, with a ratio of 74, while its affinity IC50 for 5-HT1A was 6.8 nM. The results showed the importance of an amino group in position 3 of the thienopyrimidine system for the interaction with 5-HT1A receptor binding sites, although this fragment can affect the affinity and selectivity only if linked to the

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(arylpiperazinyl)alkyl moiety. Twenty of the 30 mols. used for determining the binding affinity to 5-HT1A and alpha-adrenergic receptors were selected for QSAR anal. using a series of mol. descriptors and calculated with the TSAR software.

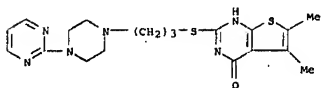
IT 185202-63-5P 185202-78-2P 185203-17-2P

185203-19-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of piperazinyl thienopyrimidinones as 5-HT1A receptor ligands)

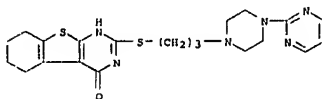
RN 185202-63-5 CAPLUS

CN Thieno[2,3-d]pyrimidin-4(1H)-one, 5,6,7,8-tetrahydro-2-[[3-[4-(2-pyrimidinyl)-1-piperazinyl]propylthio]- (9CI) (CA INDEX NAME)



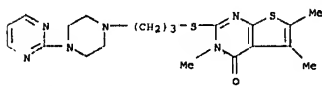
RN 185202-78-2 CAPLUS

CN [1]Benzo[thieno[2,3-d]pyrimidin-4(1H)-one, 5,6,7,8-tetrahydro-2-[[3-[4-(2-pyrimidinyl)-1-piperazinyl]propylthio]- (9CI) (CA INDEX NAME)



RN 185203-17-2 CAPLUS

CN Thieno[2,3-d]pyrimidin-4(3H)-one, 3,5,6-trimethyl-2-[[3-[4-(2-pyrimidinyl)-1-piperazinyl]propylthio]- (9CI) (CA INDEX NAME)



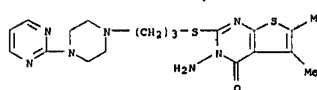
RN 185203-19-4 CAPLUS

CN Thieno[2,3-d]pyrimidin-4(3H)-one, 3-amino-5,6-dimethyl-2-[[3-[4-(2-pyrimidinyl)-1-piperazinyl]propylthio]- (9CI) (CA INDEX NAME)

&lt;12/04/2007&gt;

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REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 11 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1996:21177 CAPLUS

DOCUMENT NUMBER: 124:261075

TITLE: Preparation of 2-(piperazinylalkylthio)pyrimidines and analogs as dopamine D3 receptor ligands

PATENT ASSIGNEE(S): BASF A.-G., Germany

SOURCE: Ger. Offen., 17 pp.

CODEN: GWXXDX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 4425143	A1	19960118	DE 1994-4425143	19940715 <--
CA 2195241	A1	19960201	CA 1995-2195241	19950714 <--
WO 9602519	A1	19960201	WO 1995-EP2784	19950714 <--
W: AU, BG, BR, CA, CN, CZ, FI, HU, JP, KR, MX, NO, NZ, RU, SI, UA, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9531116	A	19960216	AU 1995-31116	19950714 <--
AU 703857	B2	19990401		
ZA 9505868	A	19970114	ZA 1995-5868	19950714 <--
EP 772603	A1	19970514	EP 1995-926898	19950714 <--
EP 772603	B1	20020612		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
CN 1152917	A	19970625	CN 1995-194141	19950714 <--
CN 1124269	B	20031015		
JP 10502659	T	19940310	JP 1996-504703	19950714 <--
JP 3819024	B2	20060906		
HU 77535	A2	19980528	HU 1997-113	19950714 <--
IL 114599	A	19990817	IL 1995-114599	19950714 <--
RU 2172736	C2	20010827	RU 1997-102159	19950714 <--
AT 2190615	T	20020615	AT 1995-926898	19950714 <--
PT 772603	T	20021129	PT 1995-926898	19950714 <--
ES 2178676	T3	20030101	ES 1995-926898	19950714 <--
CZ 295346	B6	20050713	CZ 1997-123	19950714 <--
TW 455587	B	20010921	TW 1995-84108221	19950808 <--
BG 63257	B1	20010731	BG 1997-101110	19970106 <--
FI 9700150	A	19970114	FI 1997-150	19970114 <--
NO 9700162	A	19970114	NO 1997-162	19970114 <--
NO 312030	B1	20020304		
US 6342604	B1	20020129	US 1997-765292	19970114 <--
US 6446674	B1	20020903	US 2001-940937	20010829 <--
PRIORITY APPLN. INFO.:			DE 1994-4425143	A 19940715
			WO 1995-EP2784	W 19950714
			US 1997-765292	A3 19970114

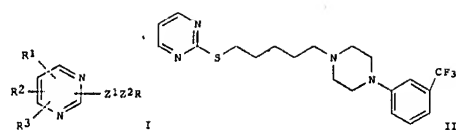
OTHER SOURCE(S): MARPAT 124:261075

&lt;12/04/2007&gt;

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10/513699

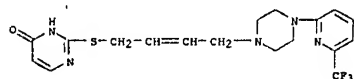
Q1



AB Title compds. [I; R = (un)substituted Ph, -pyridyl, -pyrimidyl, -triazinyl; R1-R3 = H, halo, OH, alkoxy, (di)alkylamino, etc.; Z1 = (O-, NH-, CO2-, etc.-interrupted or -terminated) alkenylene, etc.; Z2 = piperazine-1,4-diyl, piperidinylene, etc.] were prepared as dopamine D3 receptor ligands (no data). Thus, 2-mercaptopyrimidine was thioetherified by 1-bromo-5-chloropentane and the product aminated by 1-(3-trifluoromethylphenyl)piperazine to give title compound II.

IT 175156-93-1P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); GIOU (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of 2-(piperazinoalkylthio)pyrimidines and analogs as dopamine D3 receptor ligands)

RN 175156-93-1 CAPLUS  
 CN 4(1H)-Pyrimidinone, 2-[[4-[[6-(trifluoromethyl)-2-pyridinyl]-1-piperazinyl]-2-butenylthio]- (SCI) (CA INDEX NAME)



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(FILE 'HOME' ENTERED AT 11:27:18 ON 21 SEP 2007)

FILE 'REGISTRY' ENTERED AT 11:27:45 ON 21 SEP 2007

L1 STRUCTURE UPLOADED

L2 129 S L1 FULL

FILE 'CAPLUS' ENTERED AT 11:28:15 ON 21 SEP 2007

L3 15 S L2 FULL

L4 11 S L3 AND PYC2006

<12/04/2007>

Erich Leese

10/590,707

**EAST Search History**

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	223	(544/55,544/88,544/250,544/255, 544/249,544/253,514/267,514/260. 1,514/264.1,514/228.8,514/222.2). CCLS.	US-PGPUB; USPAT	OR	OFF	2007/09/21 09:42
L2	44	I1 and pyrimidine	US-PGPUB; USPAT	OR	ON	2007/09/21 09:44
L3	15	I2 and piperazine	US-PGPUB; USPAT	OR	ON	2007/09/21 09:44
L4	12	I3 and carbonyl	US-PGPUB; USPAT	OR	ON	2007/09/21 09:44
L5	12	I4 and alkyl	US-PGPUB; USPAT	OR	ON	2007/09/21 09:55
L6	280	I5 and (piperidine or pyridine) or 1, 3-oxazine or 1,3-thiazine	US-PGPUB; USPAT	OR	ON	2007/09/21 09:52